data_global

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_publ_contact_author_fax '1 864 656 6613'
_publ_contact_author_email 'shwu@clemson.edu'
_publ_requested_journal 'Inorganic Chemistry'
_publ_section_title
;
Salt-Inclusion Synthesis of Ba₂MnSi₂O₇Cl. A Novel Polar
Framework Containing Acentric [Si₂O₇]⁶⁻ Polyanion in the anti-ReO₃
Type [(Ba₂Mn)Cl]⁶⁺ Cage
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=====

CRYSTAL DATA

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;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.

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O2 0.0144(14) 0.0144(14) 0.012(2) 0.000 0.000 0.0068(19)
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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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 Ba1 O2 Ba1 91.03(16) 2_556 1_566 ?
 Si1 O3 Mn1 147.01(19) 4_545 1_545 ?
 Si1 O3 Ba1 101.12(14) 4_545 1_556 ?
 Mn1 O3 Ba1 103.39(11) 1_545 1_556 ?
 Si1 O3 Ba1 99.66(13) 4_545 3_446 ?
 Mn1 O3 Ba1 97.95(12) 1_545 3_446 ?
 Ba1 O3 Ba1 99.03(9) 1_556 3_446 ?

_diffraction_measured_fraction_theta_max	0.956
_diffraction_reflns_theta_full	30.11
_diffraction_measured_fraction_theta_full	0.956
_refine_diff_density_max	0.727
_refine_diff_density_min	-0.951
_refine_diff_density_rms	0.179